Title: **Exploratory Research on Simulation of CO_2-Brine-Mineral Interactions**

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1. Abstract

- OBJECTIVE(s)

Application of many carbon sequestration strategies requires knowledge of thermodynamic properties for extremely complex chemical systems such as, CO_2-SO_2-H_2O-NaCl-$CaCl_2$-$MgCl_2$. The objective of this research is to explore a unique approach to develop a unified equation of state (EOS) to describe thermodynamic properties in the above chemical system. We will start the research project by assessing the currently available data and models, and their appropriateness for the carbon sequestration process. We will then work on the building blocks for the unified model. CO_2 solubility models for the CO_2-H_2O-NaCl system will be updated with newly available experimental data and based on the new development in thermodynamics and molecular dynamics. This will allow computer simulations of geochemical reactions in laboratory experiments and permit upscaling to industrial and field-scale production. A coupled model based on previous models for volumetric properties in the CO_2-H_2O-NaCl system will be developed, which will allow for a better assessment of the effectiveness of CO_2 injection into deep geological formations. A strategy to address the complexity of the chemical system will be developed and this will help to meet the long-term goal of developing an EOS that is suitable for the temperature

- ACCOMPLISHMENTS TO DATE

The project has a delayed start because Chen Zhu has moved to Indiana University. A 1 year no-cost extension of the performance period was requested and approved.

- FUTURE WORK

See above

- LIST OF PAPER PUBLISHED, U.S. PATENT/PATENT APPLICATION(S), CONFERENCE PRESENTATIONS, STUDENTS SUPPORTED UNDER THIS GRANT

See above